

4-Isobutylmorpholine
10315-98-7 | DTXSID30145675

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.72 | 51.8 | 0.74 | 50.3 | 0.73 | 52.7 |

Model Results

Predicted value: -47.7 °C

Global applicability domain: Inside

Local applicability domain index: 5.77e-01

Confidence level: 5.74e-01

Nearest Neighbors from the Training Set

Image not found

4-Butylmorpholine

Measured: -57.1

Predicted: -49.8

Image not found

N-Ethylmorpholine

Measured: -64.0

Predicted: -53.3

Image not found

Piperidine, 1-acetyl-

Measured: -13.4

Predicted: -6.83

Image not found

N-Formylpiperidine

Measured: -30.8

Predicted: -13.3